

D-Phenylalanine
673-06-3 | DTXSID4025876

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 57.8 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.22e-01

Confidence level: 7.89e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>N-(3-chlorophenyl)-N'-methylurea</div> <div>Measured: 85.1</div> <div>Predicted: 101</div>	<div>Image not found</div> <div>N-Methyl-N'-phenylurea</div> <div>Measured: 19.5</div> <div>Predicted: 29.8</div>	<div>Image not found</div> <div>Urea, (3-methylphenyl)-</div> <div>Measured: 36.3</div> <div>Predicted: 37.2</div>
<div>Image not found</div> <div>Urea, (3-chloro-4-methoxyphenyl)-</div> <div>Measured: 100</div> <div>Predicted: 47.5</div>	<div>Image not found</div> <div>N-(3-chloro-4-methylphenyl)-N'-methylurea</div> <div>Measured: 126</div> <div>Predicted: 99.6</div>	